

Generalized Numerical Renormalization Group for Dynamical Quantities

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In this paper we introduce a new approach for calculating dynamical properties within the numerical renormalization group. It is demonstrated that the method previously used fails for the Anderson impurity in a magnetic field due to the absence of energy scale separation. The problem is solved by evaluating the Green function with respect to the reduced density matrix of the *full* system, leading to accurate spectra in agreement with the static magnetization. The new procedure (denoted as DM-NRG) provides a unifying framework for calculating dynamics at any temperature and represents the correct extension of Wilson's original thermodynamic calculation.

Quantum impurity models and their low-temperature properties are of central importance in condensed matter physics. They show characteristic many-body effects like the screening of a local moment by conduction electrons (the Kondo effect) which was first observed in measurements on dilute magnetic impurities in metals (see [1]). More recently, artificial nanostructures (quantum dots [2] or surface atoms probed by STM [3,4]) with tunable parameters provided new representations of the Anderson or Kondo model [5,6]. In theory, a very fruitful line of research was opened by the development of dynamical mean-field theory (DMFT) [7] where correlated lattice systems are mapped onto effective impurity models which are then accessible in a controlled way [8].

In all the above areas, progress depends sensitively on the existence of a reliable calculational method that can provide static and dynamic (spectral) properties in the full energy range. Wilson's numerical renormalization group [9] gave the first quantitative description of the Kondo effect. In systems with very different energy scales (small Kondo temperature T_K , large bandwidth) it is the only technique that can do so. In the original calculation Wilson focused on obtaining thermodynamic expectation values like the impurity susceptibility by iterative diagonalization. Each iteration step was shown to correspond to a certain temperature where expectation values could be obtained with great precision. Later, the method was extended to zero temperature dynamical properties by several groups and applied to a variety of problems [10,11], including recent DMFT calculations (e.g. [12,13]). In these calculations the additional assumption had to be made that transitions from the *ground state* to higher excitations are already correctly described in the first few iterations. Accurate results in agreement with sum rules were obtained for the single particle spectrum in the absence of external fields. In the following, however, we demonstrate that this procedure is not rigorous and fails for the Anderson impurity model in a magnetic field. To remedy the defect, we introduce a new approach based on the concept of the *reduced density matrix*. This procedure (which in the following will be denoted as DM-NRG) makes use of the full information contained in iterative diagonalization and can therefore

be considered as the true extension of Wilson's original work to dynamical quantities.

To be specific, we consider the spin 1/2 Anderson model $H = H_0 + H_{\text{imp}}$ where the impurity part is given by

$$H_{\text{imp}} = V \left(f_{\sigma}^{\dagger} c_{0\sigma} + h.c. \right) + U n_{f\uparrow} n_{f\downarrow} - \epsilon_f n_f - h S_f^z. \quad (1)$$

Here we have introduced a local magnetic field h coupled to the impurity spin S_f^z , an on-site Coulomb repulsion U , and a hybridization $\Delta = \pi V^2/2$ to the conduction band orbital $c_{0\sigma}$. Units are chosen as $\hbar = k_B = g = \mu_B = 1$. Depending on the energy of the impurity level, ϵ_f , different physical behaviour is realized. In the following, we focus on the symmetric ($\epsilon_f = -U/2$) and mixed valence ($|\epsilon_f| \approx \Delta$) regimes. The conduction band (extending in the range $[-1, 1]$) is already written in the *linear chain* representation characteristic for NRG

$$H_0 = \sum_{n=0}^{\infty} \xi_n \left(c_{n\sigma}^{\dagger} c_{n+1\sigma} + h.c. \right) \quad (2)$$

where the hopping matrix elements decay exponentially $\xi_n \sim \Lambda^{-n/2}$ due to a logarithmic discretization of the conduction band. This model – while still a nontrivial many-body problem – can now be solved by iterative diagonalization, keeping in each step only the lowest, most relevant levels. The number of iterations then corresponds to the temperature one is interested in according to $T_N = c \Lambda^{-(N-1)/2}$, where c is a constant of order one. For calculating static quantities, all necessary information is thus obtained because only excitations on the scale T_N are relevant. For dynamical properties, however, an additional energy scale is provided by the frequency ω which may be much larger than the temperature. Let us focus on the spin resolved single particle spectral density

$$A_{\sigma}(\omega) = \sum_{nm} |\langle m | f_{\sigma}^{\dagger} | n \rangle|^2 \delta(\omega - E_m + E_n) \frac{e^{-\beta E_m} + e^{-\beta E_n}}{Z} \quad (3)$$

in the Lehmann representation where the $|n\rangle$ are the many-particle eigenstates of H and Z is the partition

function. Obviously, spectral information at frequencies $\omega \gg T_N$ requires matrix elements between low-lying states and excitations which in iteration N are not available anymore (they have already been lost by truncation). To circumvent this difficulty, the following “ad hoc” procedure has been used so far: In calculating $A(\omega)$, expression (3) was simply evaluated in iteration step $N' \ll N$ where $T_{N'} \approx \omega$, assuming that for an analysis of this spectral regime the low energy levels were described well enough. There is no rigorous argument to justify this assumption, as, for example, the crossover to the strong coupling fixed point and the corresponding change in the ground state may occur at a much lower temperature scale $T_K \ll T_{N'}$.

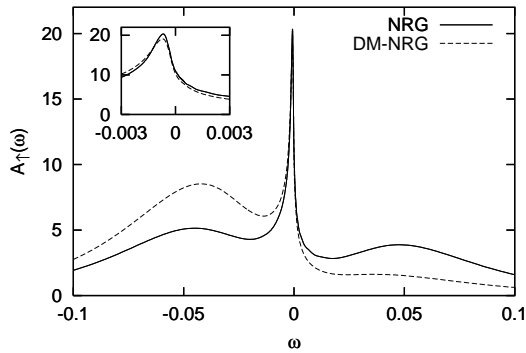


FIG. 1. Comparison of single particle spectral functions for the symmetric model ($\Delta = 0.01$, $U = 0.1$, $\epsilon_f = -0.05$) obtained by the method previously used (“NRG”) and the generalized procedure presented here (“DM-NRG”). A small magnetic field $h = 0.001$ has been applied to the impurity.

In fig. 1 we present results for the symmetric model (1) at $T = 0$ which have been calculated in this way. Without external field, one obtains the well-known three-peak structure characteristic for a small Kondo temperature T_K . Switching on a small magnetic field $h = \mathcal{O}(T_K)$ only affects the quasiparticle peak, while the high energy spectrum is almost unchanged. This result is easily understood: In the iterations where the atomic levels are calculated, the NRG procedure does not yet “know” about the tiny perturbation that eventually breaks the spin symmetry of the ground state. One can, however, easily verify that this result is incorrect: Calculating the ground-state magnetization m (a static quantity) directly as a thermodynamic expectation value $\langle\langle n_{f\uparrow} - n_{f\downarrow} \rangle\rangle$ and comparing with the value derived from the spectrum

$$m = \int_{-\infty}^0 d\omega A_{\uparrow}(\omega) - \int_{-\infty}^0 d\omega A_{\downarrow}(\omega) \quad (4)$$

the results do not agree (see table in fig. 3). Physically, the strong polarization of the impurity due to a small magnetic perturbation should suppress the upper atomic level because no particle excitations are possible anymore. This suppression is drastically underestimated by

the method used so far (indeed, in the limit of vanishing Kondo temperature T_K it will not be seen at all).

In order to capture this effect it is clearly necessary to obtain the correct ground state *before* calculating the spectra. This is achieved by the following two-stage procedure:

1) NRG iterations are performed down to the temperature T_N of interest, in particular we choose $T_N \ll T_K$ to calculate ground-state properties. In each iteration step, we keep the information on the transformation between one set of eigenstates and the next, i.e. we save the corresponding unitary matrix. After obtaining the relevant excitations at temperature T_N one can define the density matrix

$$\hat{\rho} = \sum_m e^{-E_m/T_N} |m\rangle_N \langle m| \quad (5)$$

which completely describes the physical state of the system. In particular, the equilibrium Green’s function can be written as

$$G_{\uparrow}(t) = i\theta(t)\text{Tr} \left(\hat{\rho} \left\{ f_{\uparrow}(t), f_{\uparrow}^{\dagger}(0) \right\} \right) \quad (6)$$

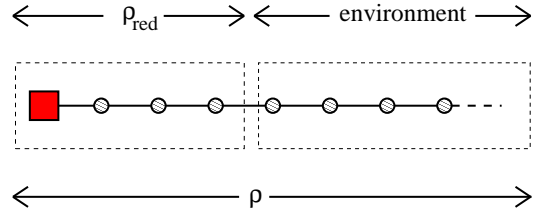


FIG. 2. Reduced density matrix obtained by tracing out “environment” degrees of freedom of the chain.

2) Now we repeat the iterative diagonalization for the same parameters. Each iteration step N' yields the single-particle excitations (and matrix elements of f^{\dagger}) relevant at a frequency $\omega \sim T_{N'}$. But instead of using (3), we now employ (6) and evaluate the spectral function with respect to the correct *reduced density matrix* [14]: As depicted in fig. 2, the complete chain is split into a smaller cluster of length N' and an *environment* containing the remaining degrees of freedom. In the product basis of these two subsystems, the full density matrix has the form

$$\hat{\rho} = \sum_{\substack{m_1 m_2 \\ n_1 n_2}} \rho_{m_1 n_1, m_2 n_2} |m_1\rangle_{\text{env}} \langle n_1|_{\text{sys}} \langle n_2| \langle m_2| \quad (7)$$

which is in general not diagonal anymore. Performing a partial trace on the environment then yields the density submatrix

$$\hat{\rho}^{\text{red}} = \sum_{n_1 n_2} \rho_{n_1 n_2}^{\text{red}} |n_1\rangle_{\text{sys}} \langle n_2| \quad (8)$$

with

$$\rho_{n_1 n_2}^{\text{red}} = \sum_m \rho_{mn_1, mn_2} \quad (9)$$

This projection is easily done using the previously stored unitary transformation matrices. Note that ρ^{red} – defined only on the shorter chain – contains all the relevant information about the quantum mechanical state of the *full* system. This concept has been applied very successfully in the density matrix renormalization group (DMRG) [15], where the projection on a smaller subsystem is essential for obtaining eigenstates of the model. In NRG, on the other hand, diagonalization can be performed directly due to the logarithmic discretization, but to describe the effect of the chain degrees of freedom on the impurity (or a small cluster) one has to determine ρ^{red} . In the following, we therefore refer to the calculational scheme presented here as DM-NRG.

In fig. 1 we compare the spectrum calculated by the DM-NRG to the one obtained with the NRG version used so far in the literature (the same number of levels has been used in both calculations). The strong shift of spectral weight due to the polarized impurity is now clearly seen, as well as a slight change in the height and shape of the quasiparticle peak. The magnetization has been calculated from (4) for different values of h and is in good agreement with the static calculation (see fig. 3). The remaining deviation of about three percent is due to an error in the total spectral weight.

h	m_{NRG}	$m_{\text{DM-NRG}}$	m_{direct}
0.0005	0.09	0.46	0.44
0.001	0.16	0.61	0.60
0.003	0.36	0.77	0.75
0.005	0.49	0.81	0.80
0.01	0.68	0.87	0.84

FIG. 3. Impurity magnetization obtained by different methods: from the spectrum (m_{NRG} vs. $m_{\text{DM-NRG}}$) and as a thermodynamic expectation value (m_{direct}). Impurity parameters are chosen as $\Delta = 0.01$ and $U = 0.1$.

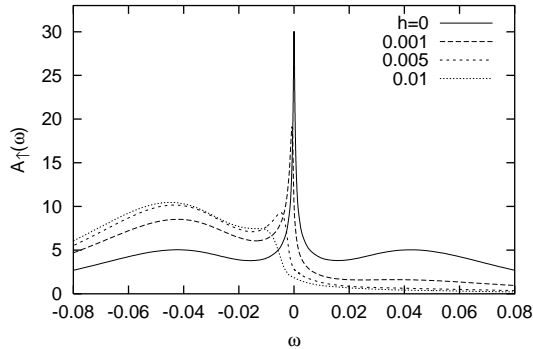


FIG. 4. Shift of the spectral function with increasing magnetic field at zero temperature. The impurity parameters are chosen as $\Delta = 0.01$ and $U = 0.1$.

The resulting field dependence of the spectrum is displayed in fig. 4. With increasing h , the Kondo resonance is suppressed and eventually merges with the lower atomic level. Regarding the total density of states (DOS) $A(\omega) = \sum_{\sigma} A_{\sigma}(\omega)$, the Kondo peak is split by the field and the DOS at the Fermi level strongly reduced. This effect has been observed directly in measurements of the differential conductance through a quantum dot [2].

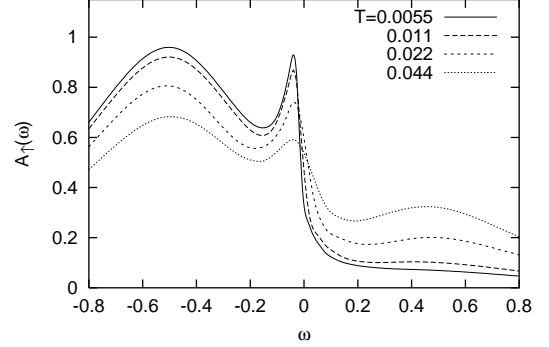


FIG. 5. Temperature dependence of the spectrum at $\Delta = 0.1$, $U = 1.0$ and $h = 0.04$. Note that at frequencies far below the temperature NRG does not yield any information. In this region the curves are fitted.

So far calculations have been at $T = 0$. Upon increase of the temperature at a finite magnetic field, we expect a reduction of the average impurity magnetization due to thermal fluctuations. As a consequence, particle excitations with polarization in the field direction should gain spectral weight. In fig. 5, this effect is obvious: At temperatures $T \gtrsim h$, the asymmetry in $A_T(\omega)$ is strongly reduced. Note that in finite temperature NRG calculations, no spectral information can be obtained at frequencies $\omega \ll T$. In this region data have to be fitted. This important fact will be discussed in detail in a subsequent publication.

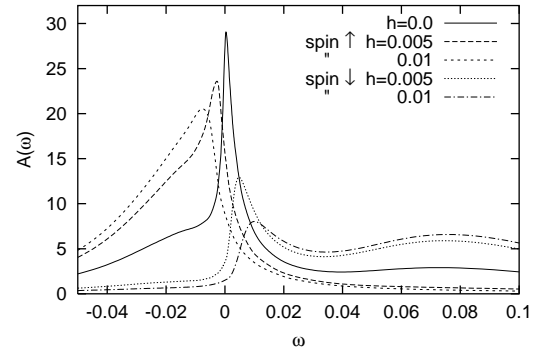


FIG. 6. Spin dependent spectral density at zero temperature for the asymmetric impurity with $\Delta = 0.01$, $U = 0.1$ and $\epsilon_f = -0.02$.

Results for an asymmetric impurity close to the mixed

valence regime are shown in fig. 6. The almost complete shift of spectral weight to the particle (hole) sector is again observed for the two spin polarizations, which in this case are not symmetric anymore. In the total DOS (fig. 7), changes are less prominent. We merely observe a suppression of the quasiparticle peak and a redistribution of the corresponding weight to higher frequencies.

Comparing our findings to previous calculations, it should be pointed out that up to now only the modified perturbation theory [16] and the Quantum Monte Carlo method (QMC) [17] have been applied to calculate the impurity spectrum in a magnetic field. The former is limited to small U , while QMC calculations have so far only been done in the mixed valence regime (and at temperatures $T \gtrsim T_K$) due to the increase in computing cost for the symmetric case. In a recent NRG calculation on the Kondo model [18], the problems discussed here did not occur due to the absence of atomic levels. Apart from these restrictions, we find qualitative agreement with our results, which do not suffer from similar limitations.

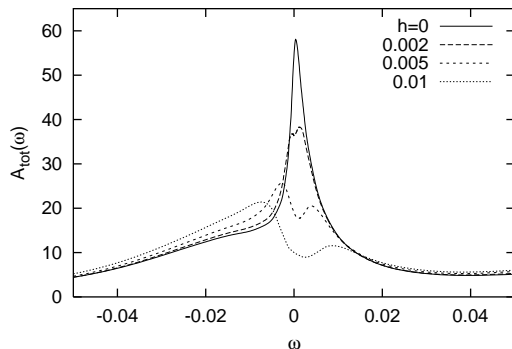


FIG. 7. Total spectral density $A_{\text{tot}} = A_{\uparrow} + A_{\downarrow}$ at zero temperature for the asymmetric impurity with $\Delta = 0.01$, $U = 0.1$ and $\epsilon_f = -0.02$. Note that upon increasing h part of the spectral weight is shifted to the upper atomic level (not shown). The total weight is constant with high accuracy.

In conclusion, we have presented a new method for calculating dynamical properties at arbitrary temperatures within the numerical renormalization group. It has been demonstrated that – despite logarithmic discretization – energy scale separation is in general not valid in the case of spectral quantities. This effect is neglected in the NRG scheme used so far in the literature. Within our generalized procedure (DM-NRG), based on the reduced density matrix, we can now account for changes in the ground state occurring at energies far below the external frequency scale.

The method introduced here has been applied to the Anderson impurity in an external magnetic field, which is of great interest in view of recent transport measurements of quantum dots. Nonperturbative $T = 0$ studies have not been performed so far, mainly because of technical difficulties in extending NRG to systems with

broken spin symmetry. Our spectral results are in excellent agreement with the sum rule provided by the (static) magnetization. In the total density of states we find the splitting and suppression of the quasiparticle peak which is also observed experimentally.

Future applications of the DM-NRG include DMFT calculations for phases with long range order, where symmetry-breaking perturbations and their effect on the spectrum have to be treated reliably. In addition, more complex impurity systems including orbital degeneracy may be studied, which (due to the rapid advances in nanoscale preparation techniques [19]) are of growing experimental interest.

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